

ABSTRACT OF THE DISCLOSURE

An approach for detecting polymers and polymer fragments by analyzing mass analysis data of mixtures that include labeled versions of the polymers is disclosed. A library of polymer fragments is generated based on the possible fragments of a parent polymer. For each fragment in the library, a theoretical mass for both a natural version and a labeled version is generated. The labeled version may be based on a heavier isotope of an element. Data from a mass analysis, such as a mass spectrographic analysis, is received and automatically analyzed to identify whether a mass doublet is observed for each fragment in the library. The mass doublets correspond to the mass peaks of the natural and labeled versions of the fragments in the library. A determination is made whether a particular mass peak is from a labeled parent polymer or whether the particular mass peak is from an unlabeled source.